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Discretely Conservative Multiphase Advection on Unstructured Meshes Using the Interface Reconstruction Library Title:

Author(s): Chiodi, Robert Michael

Intended for: Possible presentation at my home university, Cornell University.

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Discretely Conservative Multiphase Advection on Unstructured Meshes Using the Interface Reconstruction Library

Robert Chiodi

Cornell University

CCS-2 Summer Intern

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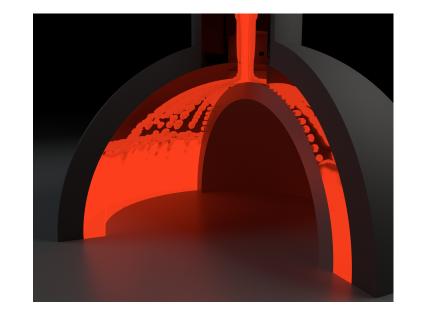




Simulates advanced metal casting processes of exotic materials

Incorporates heating of mold, injection of molten metal, and solidification.

Used as a design tool to adjust manufacturing processes.



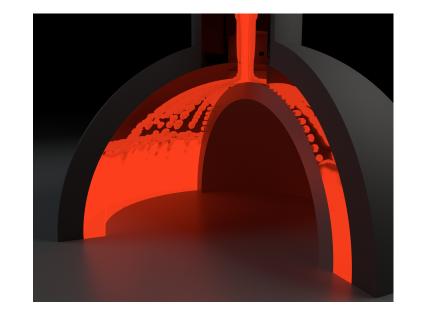




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Characteristics of Truchas Flows

- Complicated domains
- High density ratios between fluids
- Multiple materials in domain
- Multiple scalars to track (temperature, enthalpy, etc.)





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- Track multiple phases and represent multiple interfaces in one cell
- Consistent fluxing of volumes with associated scalars





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- Need to have reasonable time-to-solution.





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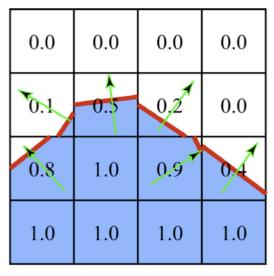
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Geometric Volume of Fluid Methods

- Work with general polyhedra
- Can couple phase volume fluxes with other fluxes (i.e. momentum, scalars)
- Multiple phases possible with onion-skin or nested-dissection
- Unconditionally stable, can use at high CFL



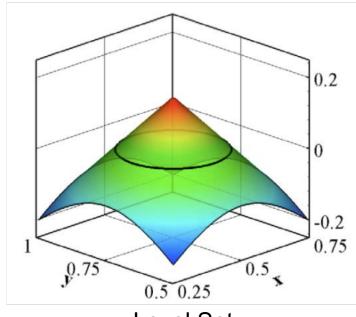




Volume of Fluid

Transport: Volume

Find: Interface

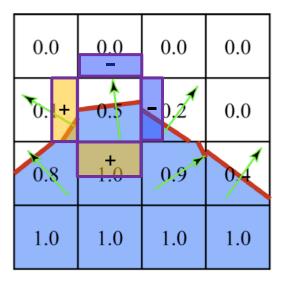


Level Set

Transport: Interface (implicitly)

Find: Volume





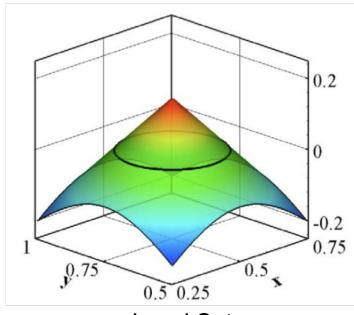
Volume of Fluid

Transport: Volume

Find: Interface

$$\alpha^{n+1} = \alpha^n + \frac{1}{V_c} \sum_f F_{\alpha}$$

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Level Set

Transport: Interface (implicitly)

Find: Volume





Geometric Advection

- Formation of flux volumes
- Intersection with the underlying mesh
- Update of cell volume moments

- Assume representation of the interface in each cell
- Orient interface representation from transported quantities
- Enforce reconstruction recovers fraction of each phase in cell





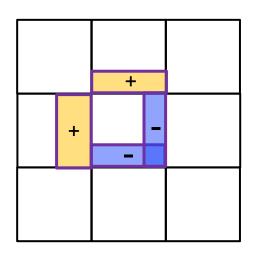
$$f_{vol} = \Delta t A_f U_f$$

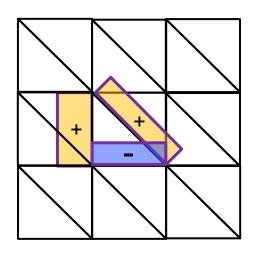
$$\alpha^{n+1} = \alpha^n + \frac{1}{V_c} \sum_f F_\alpha$$

- 1. Effectively lower time-step through using sub-steps
- 2. Iteratively modify fluxed material volumes to match total volume and preserve boundedness
- 3. Individually adjust cell face fluxes to preserve boundedness









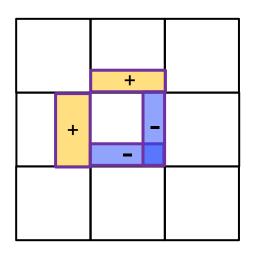
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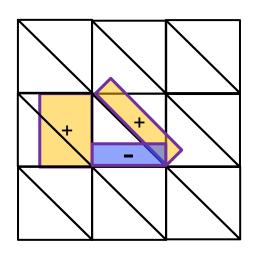
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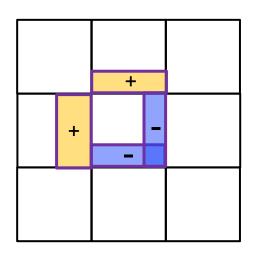
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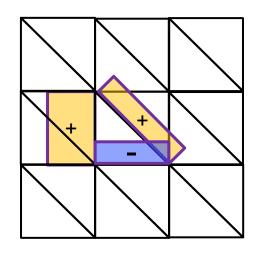
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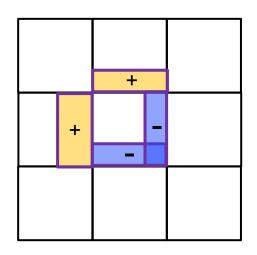
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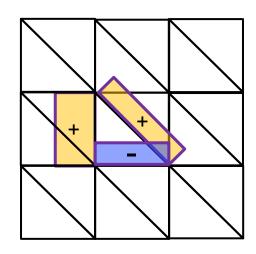
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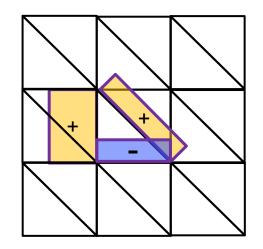
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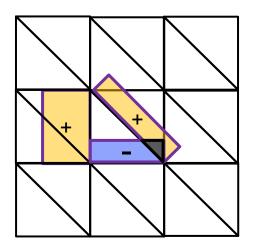




Non-Intersecting Flux Polyhedron Advection¹

$$f_{vol} = \Delta t \, A_f U_f$$





Central idea: Define priority order and do not allow volume to fluxed twice

- 1. Iterates as Truchas does to match flux volumes
- 2. Must intersect face flux polyhedral to determine if volume already taken
- 3. Results become dependent on order of face fluxing



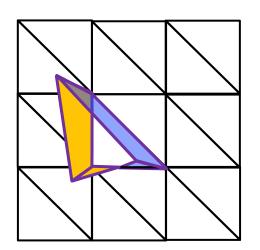


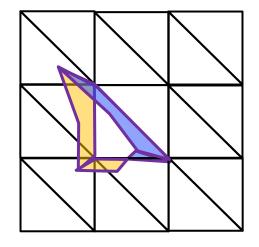
Edge-Matched Flux Polyhedron Advection

- 1. Ivey & Moin, JCP. 2017
- 2. Jofre et. al, C&F. 2014
- 3. Owkes & Desjardins, JCP. 2014
- 4. Comminal et. al, JCP. 2015

$$f_{vol} = \Delta t \ A_f U_f$$

$$\alpha^{n+1} = \alpha^n + \frac{1}{V_c} \sum_f F_{\alpha}$$





- 1. Use nodal velocities to project backwards in time and form flux polyhedron
- 2. Correct polyhedron to match expected volume flux





Geometric Advection

- Formation of flux volumes
- Intersection with the underlying mesh
- Update of cell volume moments

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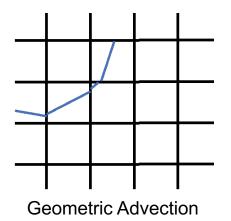
Complicated and expensive computational geometry problems

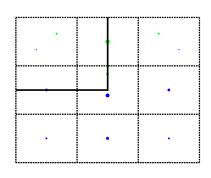
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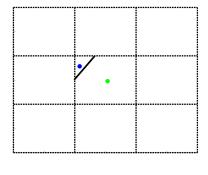


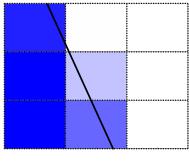


Goal: Enable wider adoption of geometric transport schemes and algorithms requiring complex computational geometry









R2P Reconstruction

MoF Reconstruction

ELVIRA Reconstruction







What do these operations require?

Obtaining some moments for the intersection between some volume and a space enclosed by some planes.

some volume

- A polyhedron or polygon
- Computational cells, flux volumes, bounding boxes, supercells,...

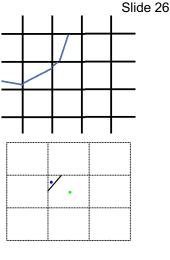
some planes

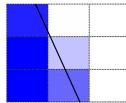
- A collection of n-planes in 3D that partition Euclidean space
- ➤ Cell boundaries, liquid-gas interfaces, arbitrary convex 2/3-polytopes,...

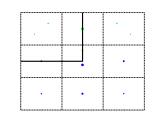
some moments

- Moments from integrating over the intersection of some volume and the space enclosed by some planes
- Volume, centroid, face normal vector,...

IRL provides high-performance, general algorithms usable for structured, unstructured, and AMR frameworks





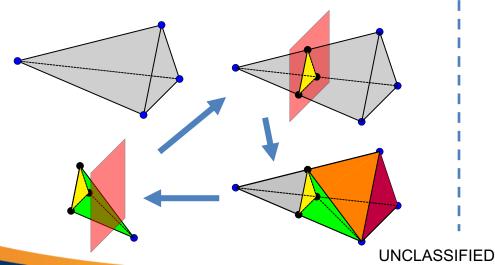




Available Volume Intersection Methods

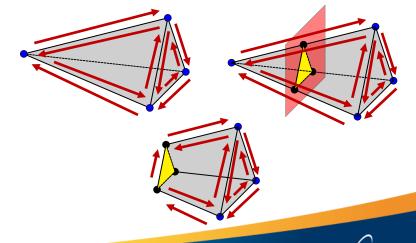
Recursive Simplex

- 1. Decompose a polytope into set of simplices
- 2. Intersect each simplex with the plane(s)
- 3. Sum up contribution to the volume moments



Half-Edge Clip & Cap

- 1. Transform polytope to half-edge structure
- 2. Clip & Cap half-edge structure
- 3. Compute volume moments through face triangulation



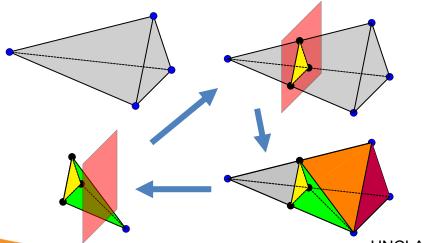




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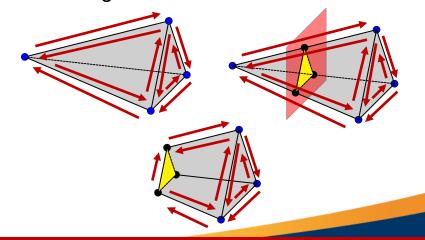
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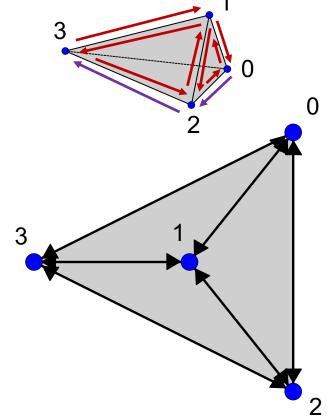






Half-Edge Structures

A typical representation of a polytope might include vertices, edges, and faces. The edges form a bi-directional undirected graph for the vertices



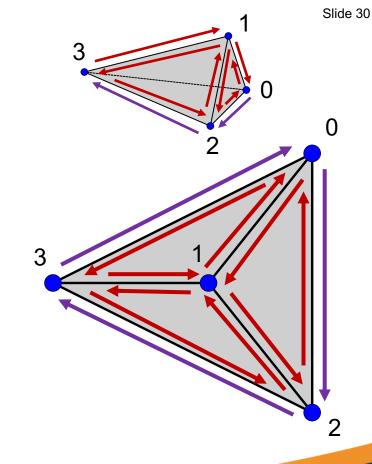






A typical representation of a polytope might include vertices, edges, and faces. The edges form a bi-directional undirected graph for the vertices.

A half edge structure represents the polytope with a directed graph of the vertices. Each edge is represented by two directed half edges.









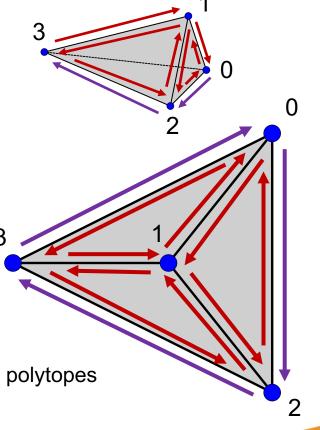
Half-Edge Structures

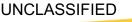
Important half-edge structure properties

- 1. Face consists of a close loop of half-edges
- Each half-edge has a mirror half edge that exists on the face sharing that edge
- 3. Known traversal direction for the face

This provides

- 1. Easy traversal of faces, vertices, and edges
- 2. Ability to calculate moments for convex and non-convex polytopes
- 3. Increased efficiency for volume intersection operations







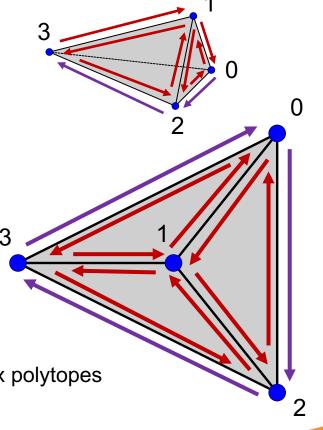
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Half-Edge Structures – Implementation

HalfEdge

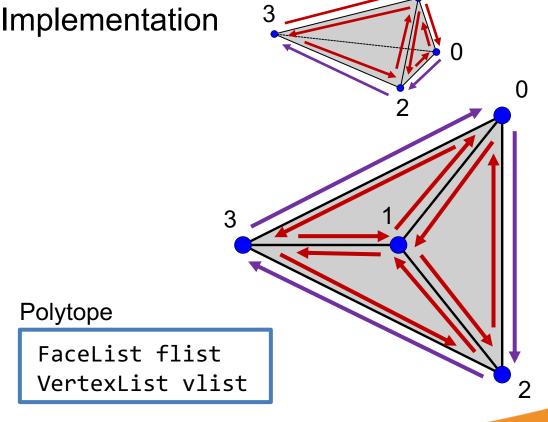
HalfEdge* previous
HalfEdge* next
Face* my_face
Vertex* edge_end

Vertex

Pt location HalfEdge* any_half_edge

Face

HalfEdge* any_half_edge



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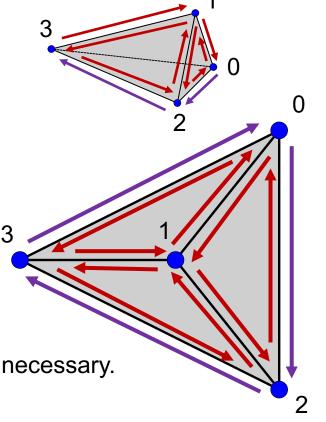


Half-Edge Structures - Clip & Cap

General algorithm

- 1. Calculate distance to vertices from plane
- 2. Find intersections and subdivide edges
- 3. Truncate each intersected face
- 4. Generate new faces on clip plane
- 5. Cleanup face and vertex list

Half edge structure provides all connectivity information necessary. Allows for fast intersection of any polytope with a plane.



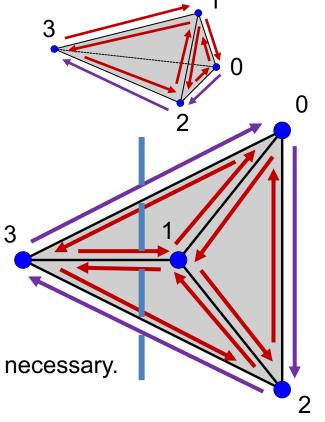




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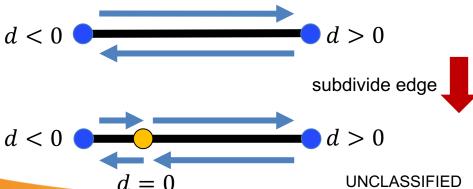


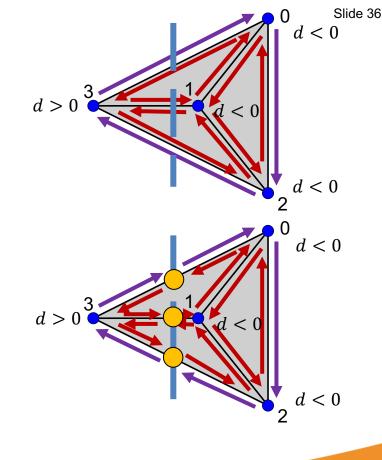




Find intersections and subdivide edges

- 1. Mark vertices with d > 0 to be clipped
- Loop over all vertices marked for clipping
 - a) Look at edges connected to neighboring vertices
 - b) If intersection found, subdivide the edge
 - c) Set vertex's half edge as new half edge

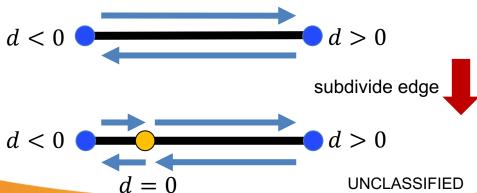


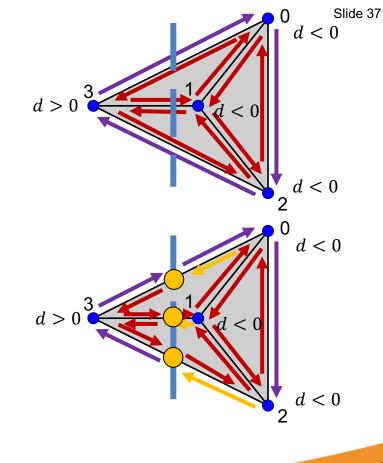




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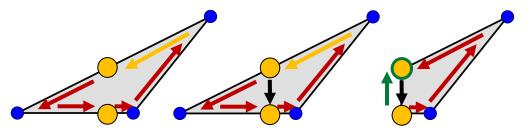


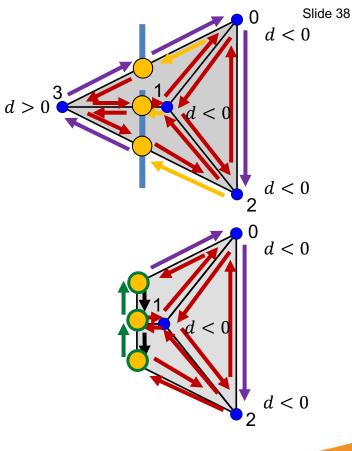


Truncate each intersected face

Loop over all new vertices

- a) Traverse face until finding next new vertex
- b) Make new half edge between two new vertices
- c) Create a mirror half edge for new half edge
- d) Set starting vertex's half edge as new mirror







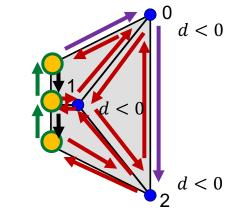


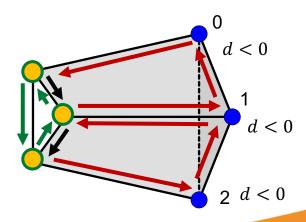
Generate new faces on clip plane

Loop over all new vertices

- a) If vertex has not been visited, take half edge
- b) Create a new face and add to list

```
Link all half edges on face
current half edge = starting half edge
do
    half edge.vertex.visited = true
    opposite half edge =
        current half edge.opposite
    previous vertex = opposite half edge.vertex
    current half edge.previous =
        previous vertex.half edge
    previous vertex.half edge =
        current half edge
    current half edge =
        current half edge.previous
while (current half edge != starting half edge)
```









Clip & Cap Performance

Intersection of random planes with polyhedron

Generate m random planes, for $m \in [1,5]$

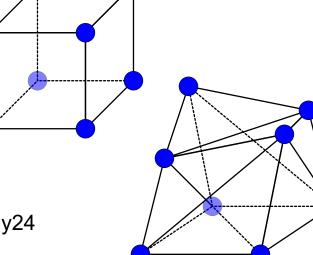
- random normal \hat{n}
- Distance in range [-0.1,0.1]

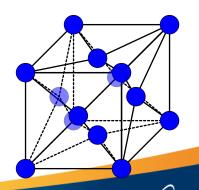
Polyhedrons intersected: Unit Cube, Dodecahedron, Poly24

All centered around the origin [0,0,0]

Intersection of two polyhedra

Two random tetrahedra with vertices on the unit sphere
Two random axis-aligned cuboids with vertices on random spheres





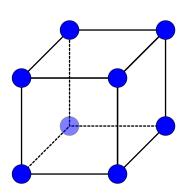


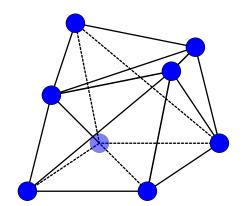


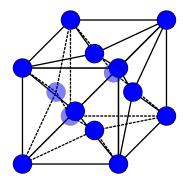
Clip & Cap Performance

R3D

- C Library to perform intersection of polyhedra with planes
- Based on simplification of half-edge structure to a three-vertex connected graph
- Provides routines for voxelization of polyhedral to rectangular grid











Timing in milliseconds / 10⁶ trials

Clip & Cap Performance

Unit Cube Intersections

m	IRL	R3D	IRL/ R3D
1	649	1320	0.49
2	1240	1890	0.66
3	1790	2300	0.78
4	2260	2620	0.86
5	2660	2840	0.94

Dodecahedron Intersections

m	IRL	R3D	IRL/ R3D
1	1050	2160	0.49
2	1970	2800	0.70
3	2500	3260	0.77
4	3070	3850	0.80
5	3520	3740	0.94

Poly24 Intersections

m	IRL	R3D	IRL/ R3D
1	1500	3860	0.39
2	3040	4410	0.69
3	3550	4550	0.78
4	4530	4590	0.99
5	5250	5370	0.98

Two polyhedra intersections

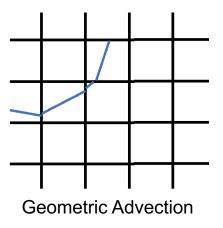
Intersection Type	IRL	R3D	IRL/ R3D
Tet-Tet	2030	2170	0.94
Cuboid-Cuboid	1220	1400	0.87





Relevant in many fields

- Geometric advection in multiphase flow simulations
- Conservative grid remapping schemes
- Voxelization in graphics

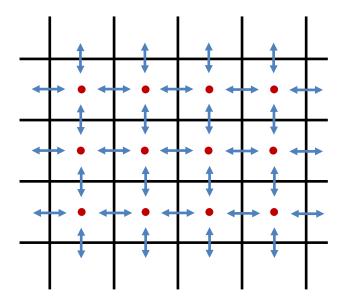


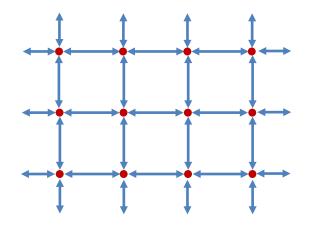
Implemented in IRL with planar reconstructions as nodes in a graph

- Capable of representing any mesh of convex cells
- Includes information on volume attributed to each node



Distribution of Volume onto a Mesh Using Reconstruction Links

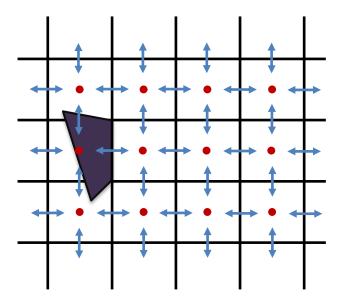


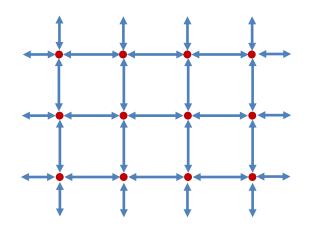






Distribution of Volume onto a Mesh Using Reconstruction Links

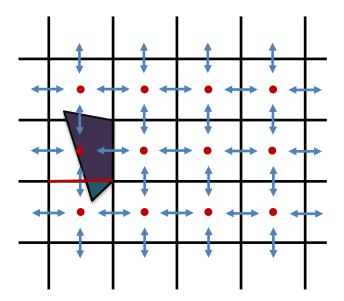


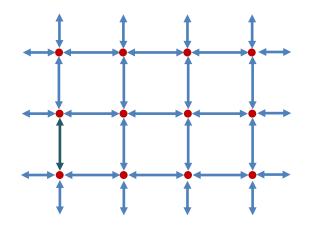






Distribution of Volume onto a Mesh Using Reconstruction Links

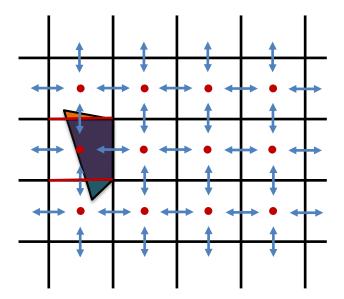


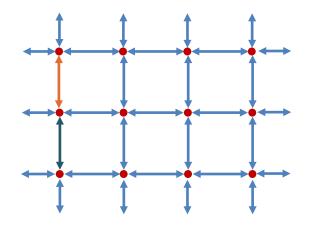






Distribution of Volume onto a Mesh Using Reconstruction Links

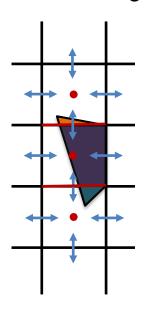


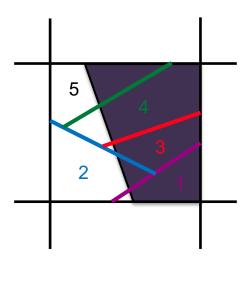


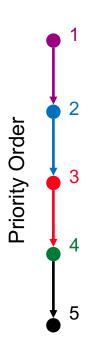




Dividing of Volume into Multiple Materials
Using Reconstruction Links







Directed Path Graph
Connecting
Reconstructions

Performing nested dissection uses the same algorithms





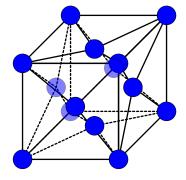
Voxelization Performance

Intersection of polyhedron onto a mesh

- Intersect with a cubic mesh in domain $[-1,1]^3$
- Mesh resolved by 3 cells in each direction
- For r3d, use r3d voxelize routine

Polyhedra intersected:

- Random tetrahedron with vertices on unit sphere
- Random cuboid with vertices on unit sphere
- Concave Poly24 randomly translated in range [-0.5,0.5]



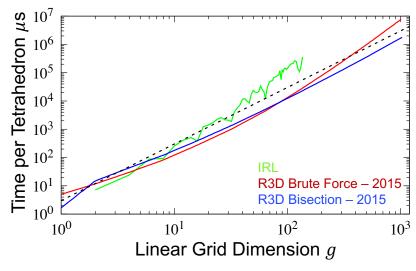


Voxelization Performance

Intersection of polyhedron onto a mesh

Intersection Type	IRL	R3D	IRL/ R3D
Tetrahedron	13670	30560	0.45
Cuboid	9550	16550	0.58
Poly24	8920	67070	0.13

Timing in milliseconds / 106 trials



*IRL averaged over 104 trials





Interface Reconstruction Library (IRL)

IRL provides a robust, efficient, and general volume intersection algorithm

- Works for polyhedra and polygons
- No inherent limit on number of vertices, faces, or half edges
- Planes can be linked together to form a graph for efficient local mesh intersection

Other features of IRL

- Contains interface reconstruction methods: LVIRA, MoF, R2P, Advected Normals
- Volume conservation enforcement for planar reconstructions
- General root finding and optimization framework

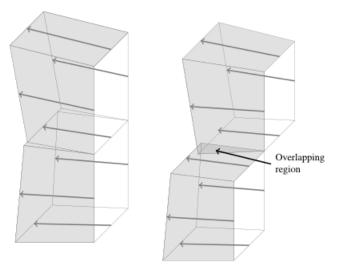


Efficient Conservative Unsplit Advection for Unstructured Meshes





Using edge velocity (overlapping and gaps)

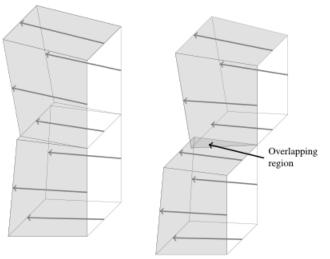


Owkes & Desjardins. JCP, 2014



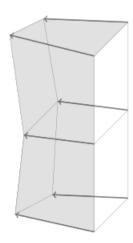


Using edge velocity (overlapping and gaps)



Owkes & Desjardins. JCP, 2014

Using node velocity (fixed overlapping/gaps)

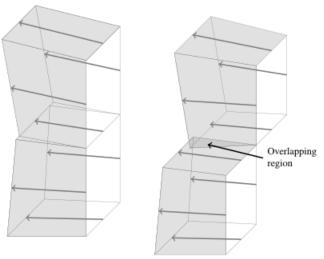






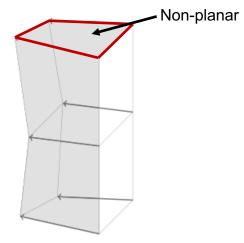


Using edge velocity (overlapping and gaps)



Owkes & Desjardins. JCP, 2014

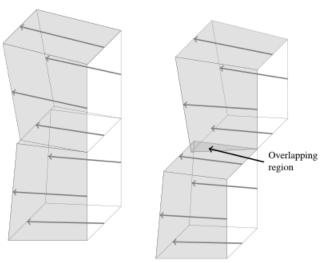
Using node velocity (fixed overlapping/gaps) (non-planar faces)





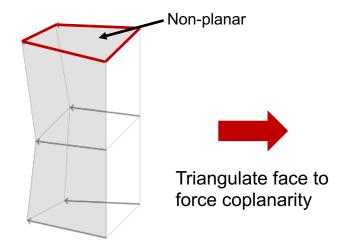


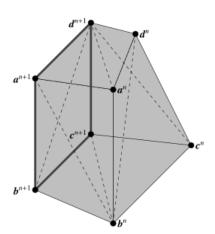
Using edge velocity (overlapping and gaps)



Owkes & Desjardins. JCP, 2014

Using node velocity (fixed overlapping/gaps) (non-planar faces)





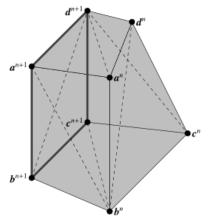
Owkes & Desjardins. JCP, 2014





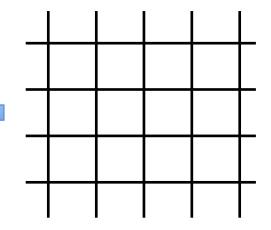


Imposed triangulation

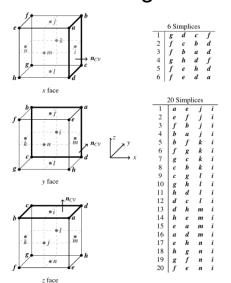


Owkes & Desjardins. JCP, 2014

Structured mesh



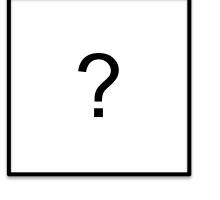
Pre-tabulated vertex orderings



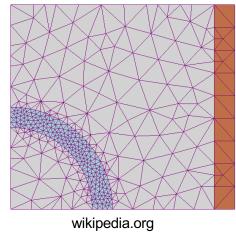




Imposed triangulation



Unstructured mesh









Truchas has four types of elements

- 1. Tetrahedron
- 2. Pyramid
- 3. Wedge (Triangular Prism)
- 4. Hexahedron

All of these have faces with 3 or 4 vertices

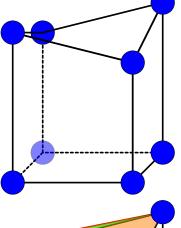
flux volumes with 6 or 10 vertices

In general, the faces of the flux volumes are **NOT** coplanar

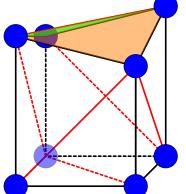


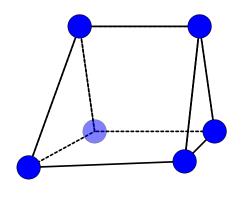


Invalid Hexahedron

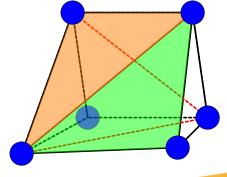


Valid Dodecahedron





Invalid Wedge



Valid Octahedron

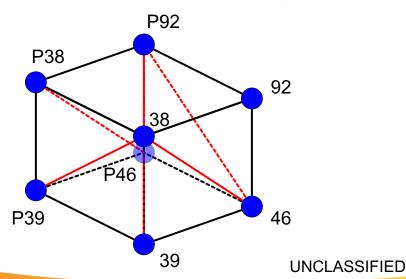






- 1. Triangulation is necessary to force coplanarity
- 2. Triangulation itself is arbitrary

Choice: Diagonalize projected edge faces based on ascending global node id

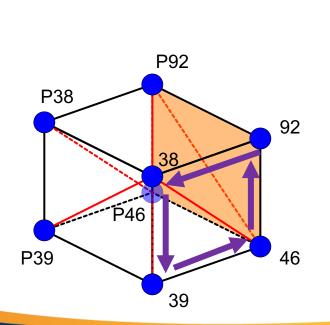


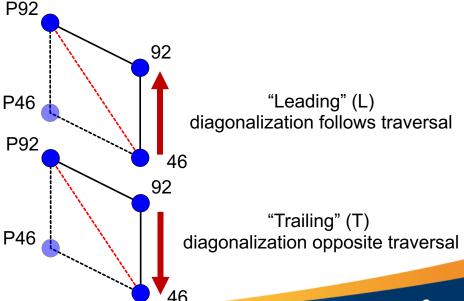




Flux volumes must be constructed from known face triangulations

Codify the face diagonalization relative to the traversal of the face







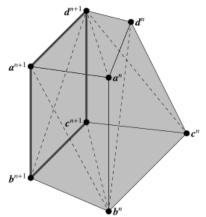
Ten categories of flux polyhedra result from this codification

Octahedron	Dodecahedron
LLL	LLLL
LLT	LLLT
LTT	LTLT
TTT	LLTT
	LTTT
	TTTT



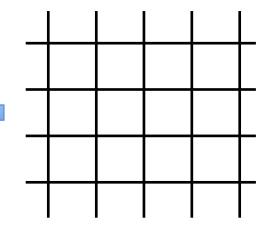


Imposed triangulation

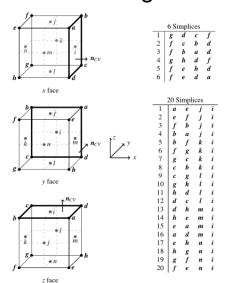


Owkes & Desjardins. JCP, 2014

Structured mesh

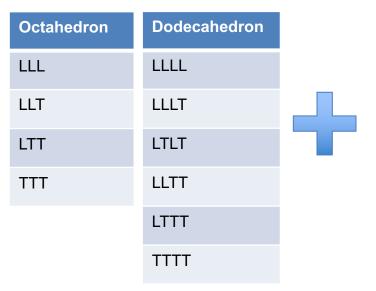


Pre-tabulated vertex orderings

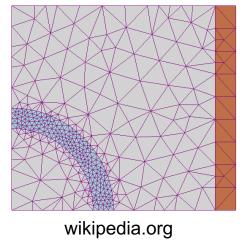




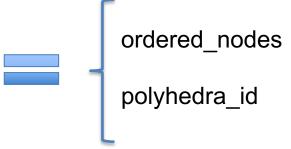
Imposed triangulation



Unstructured mesh



Vertex Ordering Set at Initialization





Classification of flux volumes types only depends on mesh elements and connectivity

- Can be performed during initialization, limited impact on performance
- General idea applicable for achieving conservative fluxing with any element geometry
- Cases can be further reduced if allow for reversal of face traversal (Reduces to six cases)

Matching of flux volume to a given amount handled by pyramidal correction

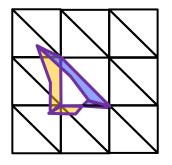
- Back projected face triangulated to a central point to find a "cap"
- Central point then adjusted to achieve desire volume
- Many options on deciding the line the central point is adjusted along
- 1. Owkes & Desjardins, JCP. 2014
- 2. Comminal et. al, JCP. 2015
- 3. Maríc et. al, JCP. 2018
- 4. Jofre et. al, C&F. 2014

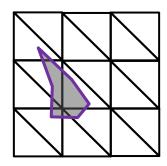




Cell-wise advection of volume fraction^{1,2}

- Direct formation of final volume entering cell
- Reduces number of intersections on mesh.
- Creates larger, better behaved polyhedra





Refinement of geometric advection band³

- Major cost is intersections with the mesh
- Approximates intersections with axis-aligned bounding boxes
- Fast and efficiently determines if intersection needed
- 1. Comminal et. al, JCP. 2015
- 2. Zhang, SIAM Num. Analysis. 2013
- 3. Maríc et. al, JCP. 2018





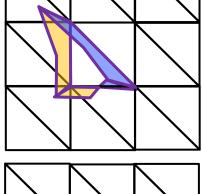
Cell-wise advection of volume fraction

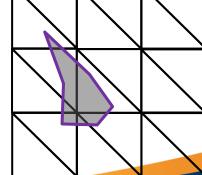
$$\frac{\partial \alpha}{\partial t} + \nabla \cdot (\alpha \vec{u}) = 0 \qquad \qquad \qquad \alpha^{n+1} = \alpha^n + \frac{1}{V_c} \sum_f F_{\alpha}$$

$$\alpha^{n+1} = \frac{1}{V_c} \left(P_{\Delta t}(C) \cap R_{\alpha} \right)$$

<u>Algorithm</u>

- 1. Back project cell vertices
- 2. Construct face fluxes (with correct face triangulation)
- 3. Correct face flux polyhedron to match given flux volume
- 4. Form corrected advected cell using projected vertices and correction vertices
- 5. Intersect corrected advected cell with mesh

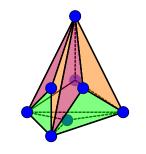




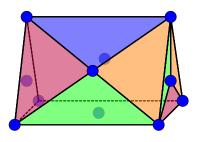
- 1. Comminal et. al, JCP. 2015
- 2. Zhang, SIAM Num. Analysis. 2013



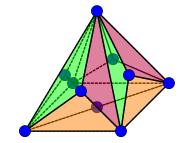
Cell-wise advection of volume fraction



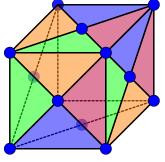
FP Tetrahedra



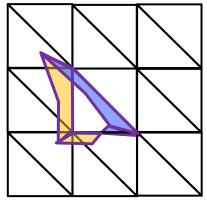
FP Wedge

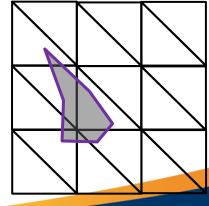


FP Pyramid



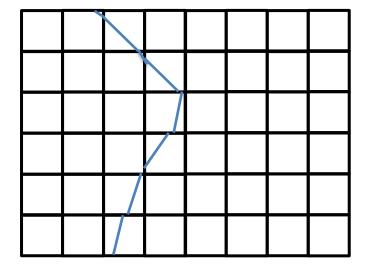
FP Hexahedron







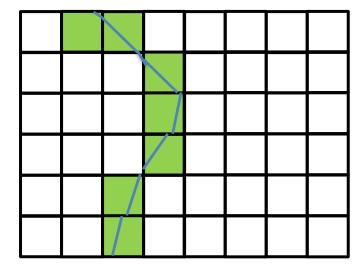
Refinement of geometric advection band





Refinement of geometric advection band

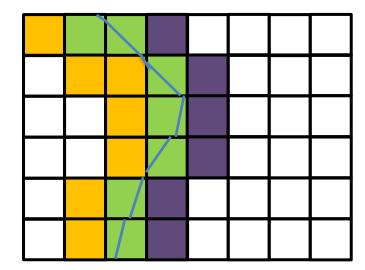
Band 0





Refinement of geometric advection band

Band 0
Band +1
Band -1





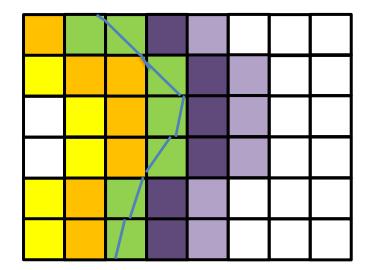
Refinement of geometric advection band

Band 0
Band +1

Band -1

Band +2

Band +2





Refinement of geometric advection band

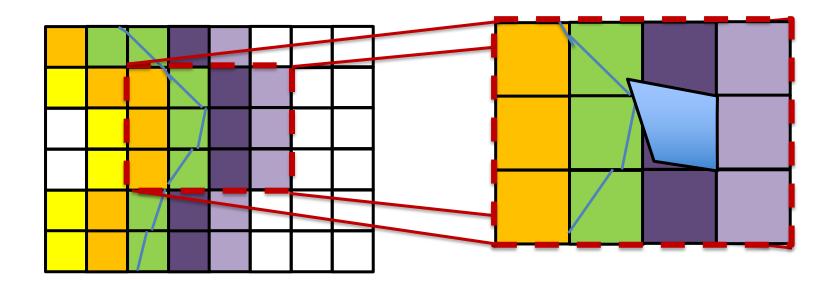
Band 0

Band +1

Band -1

Band +2

Band +2







Refinement of geometric advection band

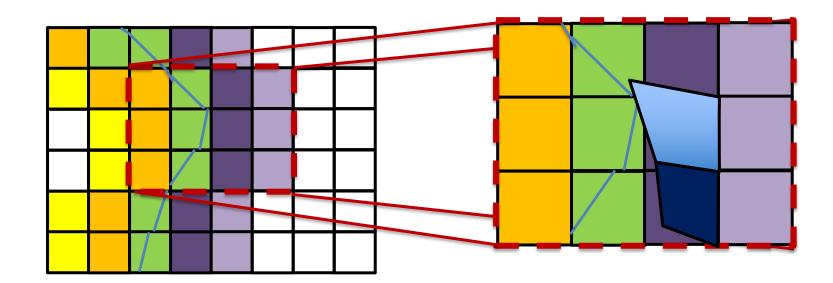
Band 0

Band +1

Band -1

Band +2

Band +2







Refinement of geometric advection band

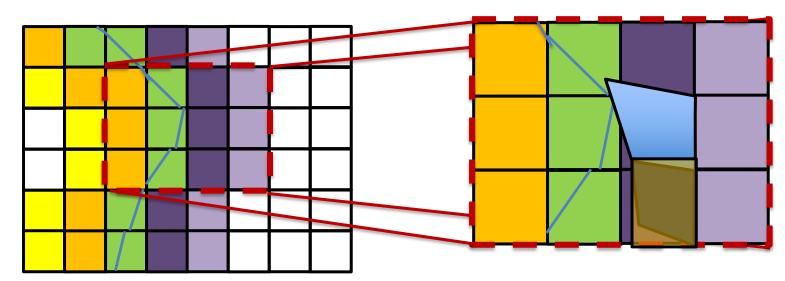
Band 0

Band +1

Band -1

Band +2

Band +2



Does sign of band change?





Refinement of geometric advection band

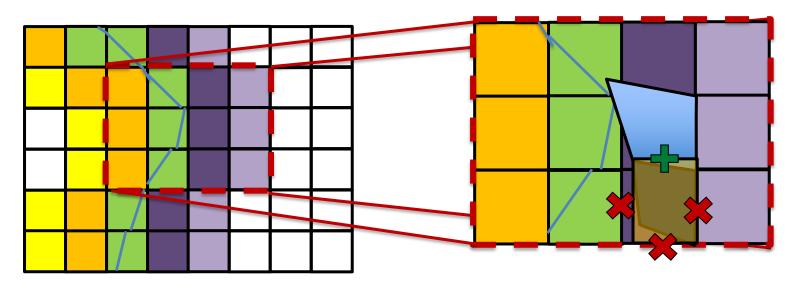
Band 0

Band +1

Band -1

Band +2

Band +2



Does sign of band change?





Refinement of geometric advection band

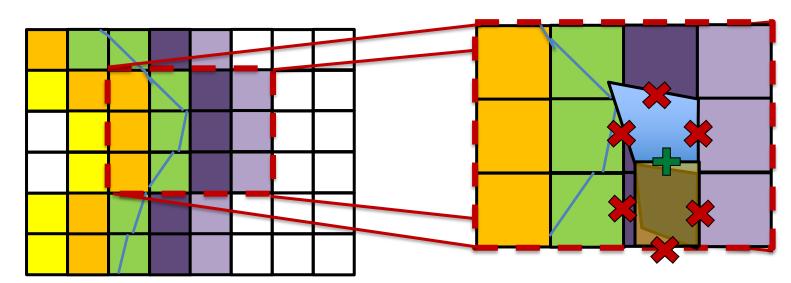
Band 0

Band +1

Band -1

Band +2

Band +2



Does sign of band change?

NO → single-phase flux

UNCLASSIFIED





Refinement of geometric advection band

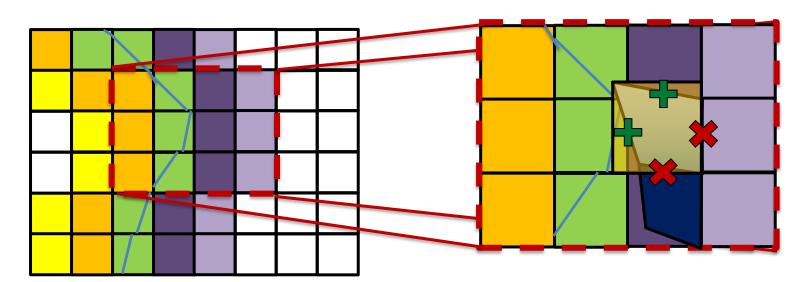
Band 0

Band +1

Band -1

Band +2

Band +2



Does sign of band change?

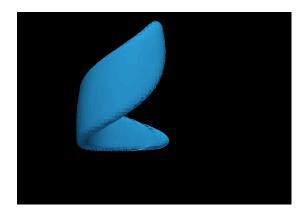
YES → multi-phase flux

UNCLASSIFIED

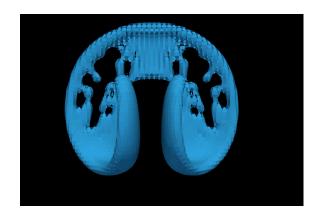




3D Shear Case



3D Deformation Case



Performance measures

$$E_g = \frac{\sum (\alpha_{initial} - \alpha_{final})V}{\sum V}$$

$$E_{v} = \sum \alpha_{initial} V - \sum \alpha_{final} V$$

$$T_{cost} = \frac{T_{wall}}{n_{steps}}$$





3D Shear Case

Prescribed reversing velocity field

$$u(\vec{x},t) = \sin(2\pi y)\sin^{2}(\pi x)\cos(\pi t/3) v(\vec{x},t) = -\sin(2\pi x)\sin^{2}(\pi y)\cos(\pi t/3)$$

$$w(\vec{x},t) = \left(1 - \frac{r}{R}\right)^2 \cos(\pi t/3), \ r = \sqrt{(x - 0.5)^2 + (y - 0.5)^2}, \ R = 0.5$$

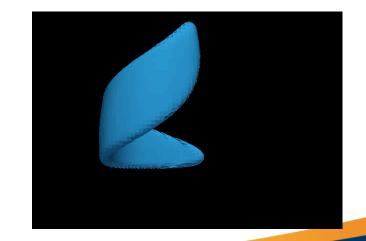
<u>Domain</u>

Dimensions $[0,0,0] \times [1,1,2]$

Discretized uniformly by $N \times N \times 2N$ hexahedron cells Simulations performed at CFL of 0.5

Initial Shape

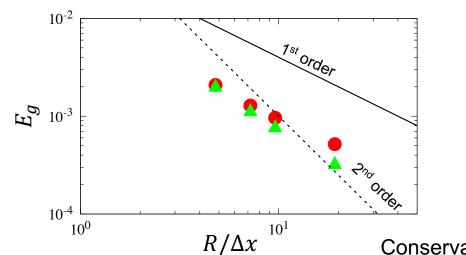
Sphere of radius 0.15, centered at (0.5, 0.75, 0.25)

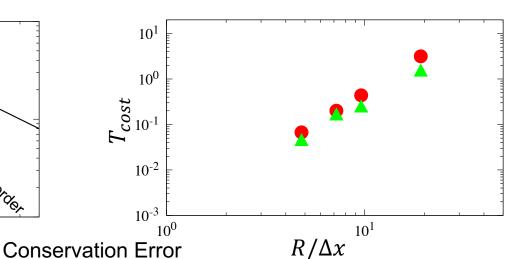


1. Liovic et. al, C&F. 2006



3D Shear Case





Old Method (Youngs)

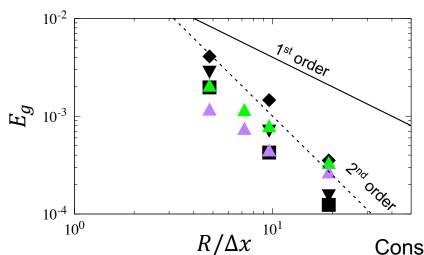
New Transport (Youngs)

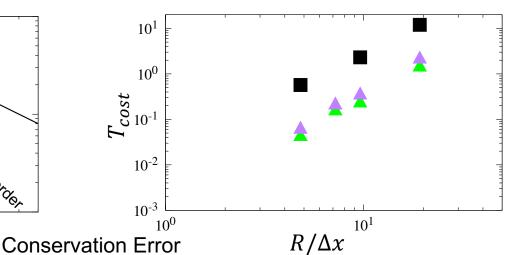
Resolution	New	Old
4.8	+1.076E-16	-1.943E-16
7.2	-3.530E-15	+5.221E-16
9.6	+1.298E-15	+1.998E-15
19.2	+1.499E-15	+5.637E-10





3D Shear Case



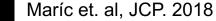


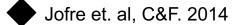
New Transport (Youngs)

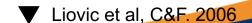
New Transport (Swartz)

331.331 741.31			
Resolution	New (Swartz)	Maríc et. al	
4.8	+3.315E-15	2.33E-15	
7.2	-4.306E-15	-	
9.6	+2.469E-15	4.91E-15	
19.2	-1.504E-15	1.22E-14	













3D Deformation Case

$$u(\vec{x},t) = \sin(2\pi y)\sin^2(\pi x)\sin(2\pi z)\cos(\pi t/3)$$
 Prescribed reversing
$$v(\vec{x},t) = -\sin(2\pi x)\sin^2(\pi y)\sin(2\pi z)\cos(\pi t/3)$$
 velocity field
$$w(\vec{x},t) = -\sin(2\pi x)\sin(2\pi y)\sin^2(\pi z)\cos(\pi t/3)$$

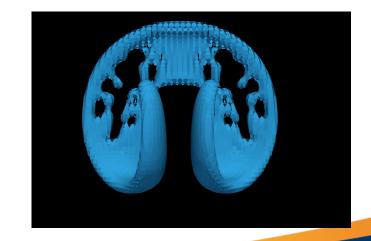
Domain

Dimensions $[0,0,0] \times [1,1,1]$

Discretized uniformly by $N \times N \times N$ hexahedron cells Simulations performed at CFL of ~0.5

Initial Shape

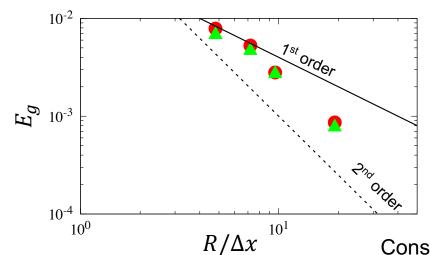
Sphere of radius 0.15, centered at (0.35, 0.35, 0.35)

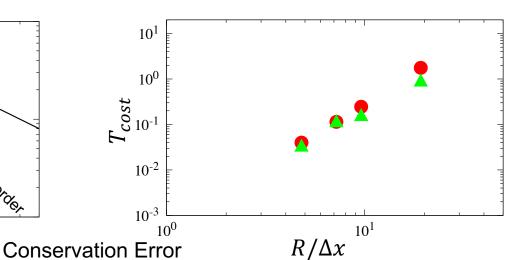


1. Enright et. al, JCP. 2002



3D Deformation Case - Hex





Old Method (Youngs)

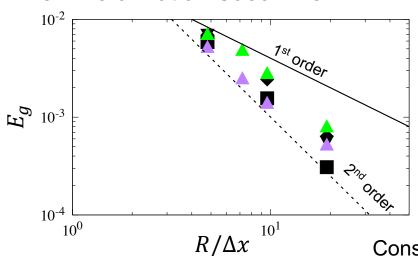
New Transport (Youngs)

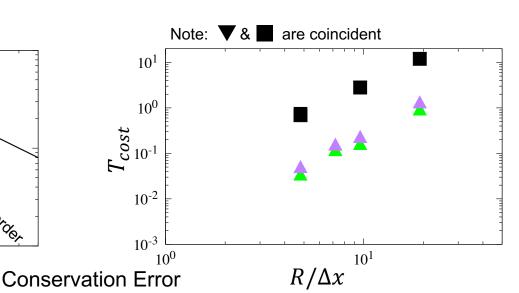
Resolution	New	Old
4.8	+4.077E-16	-2.342E-16
7.2	+5.135E-16	-2.949E-17
9.6	+8.795E-16	+2.307E-16
19.2	-6.811E-16	+2.841E-11











New Transport (Youngs)

New Transport (Swartz)

Resolution	New (Swartz)	Maríc et. al
4.8	-8.014E-16	2.46E-16
7.2	-3.296E-16	-
9.6	+2.307E-16	6.01E-15
19.2	+3.227E-16	1.56E-14



Maríc et. al, JCP. 2018



Jofre et. al, C&F. 2014

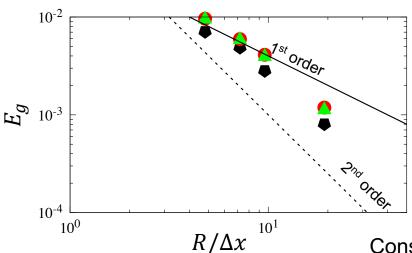


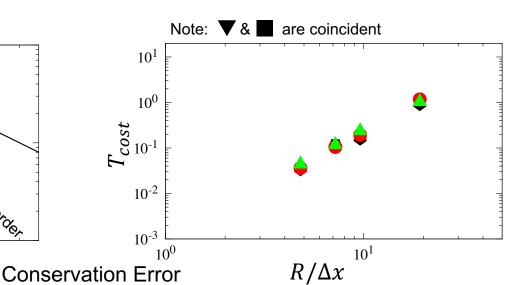
Owkes & Desjardins, JCP. 2014











Old Method (Youngs)

New Transport (Youngs)

Resolution	New	Old
4.8	-2.018E-14	-4.539E-13
7.2	-8.342E-15	-4.023E-13
9.6	8.014E-16	-4.793E-13
19.2	-6.287E-13	-4.377E-09



$$\Delta x_{tet}^3 \approx 6\sqrt{2} \, \Delta x_{hex}^3$$





Conclusions

<u>IRL</u>

- Library of computational geometry algorithms useful for unsplit VOF applications
- Robust, efficient, and general volume intersections routines
- Flexible voxelization framework for networks on convex volumes

Unsplit Advection in Truchas

- Efficient algorithm for efficient, discretely conservative geometric advection on unstructured meshes
- Imposes consistent face triangulation without centroid-based face decomposition
- Cell-wise advection and refinement of geometric advection band are two useful improvements to unsplit volume fraction methods





QUESTIONS?

UNCLASSIFIED

